<Bioinformatics Center> Bioknowledge Systems

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– Bioknowledge Systems –

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Visitors

Assoc Prof HUANG, Xin-an — Guangzhou University of Chinese Medicine, China, P. R., 4 October 2009–30 September 2010
Assist Prof RAMIREZ-PRADO, Jorge H — Scientific Research Center of Yucatan (CICY), Mexico, 7 June–31 August 2010

Scope of Research

The proteins responsible for biosynthesis, biodegradation, and transport of additional molecules, such as small metabolites, lipids and glycans, are encoded in the genome, which may indicate that all cellular functions are specified by the genomic DNA sequence. In practice, however, inferring higher-level systemic functions of the cell or the organism needs more than solely the genomic information. We are developing bioinformatics methods to integrate different types of data and knowledge on various aspects of the biological systems towards basic understanding of life as a molecular interaction/reaction system and also toward practical applications in medical and pharmaceutical sciences.

KEYWORDS

KEGG
(Meta)genomics
Pathway
Bioinformatics
Metabolomics

Selected Publications

Hattori M, Tanaka N, Kanehisa M, Goto S: SIMCOMP/SUBCOMP: Chemical Structure Search Servers for Network Analyses, *Nucleic Acids Res.*, **38,** W652-W656 (2010).

Moriya Y, Shigemizu D, Hattori M, Tokimatsu T, Kotera M, Goto S, Kanehisa M: PathPred: An Enzyme-catalyzed Metabolic Pathway Prediction Server, *Nucleic Acids Res.*, **38,** W138-W143 (2010).

Diez D, Hayes N, Joannin N, Normark J, Kanehisa M, Wahlgren M, Wheelock CE, Goto S: varDB: A Database of Antigenic Variant Sequences — Current Status and Future Prospects, *Acta Trop.*, **14,** 144 (2010).

Kanehisa M, Goto S, Furumichi M, Tanabe M, Hirakawa M: KEGG for Representation and Analysis of Molecular Networks Involving Diseases and Drugs, *Nucleic Acids Res.*, **38,** D355-D360 (2010).

Wheelock CE, Wheelock AM, Kawashima S, Diez D, Kanehisa M, van Erk M, Kleemann R, Haeggstrom JZ, Goto S: Systems Biology Approaches and Pathway Tools for Investigating Cardiovascular Disease, *Mol. Biosyst.*, **5,** 588-602 (2009).

RCLASS: Reaction Class Database

Recent development of high-throughput measurement techniques has put omics research (genomics, proteomics, metabolomics, etc.) forward to analysis on organism communities. For example, next-generation sequencers are expected to be powerful to analyze environmental genomics, also referred to as "metagenomics". Similarly, high-throughput mass spectrometry enables to analyze metabolomics on organism communities, referred to as "meta-metabolomics".

Our future goal is the integration of metagenomics and meta-metabolomics, i.e., linking metagenomic information to the interconversion among the chemical substances from environment. We developed the E-zyme software for the initial step to elucidate enzymes for a partial reaction equation. E-zyme is reaction types named as the RDM chemical transformation patterns. Specific RDM patterns are uniquely and preferentially found in specific categories of the KEGG metabolic pathways. We developed KEGG RCLASS database, classification of reactions based on the RDM patterns of reactions on metabolic pathways. One can consider the relationships between enzyme reaction similarity and enzyme protein similarity even the reaction equation is only partially identified, thus RCLASS is proposed to be beneficial to link meta-metabolomics to metagenomics, as well as to analyze consecutive reaction patterns conserved in the evolution of metabolic pathways.

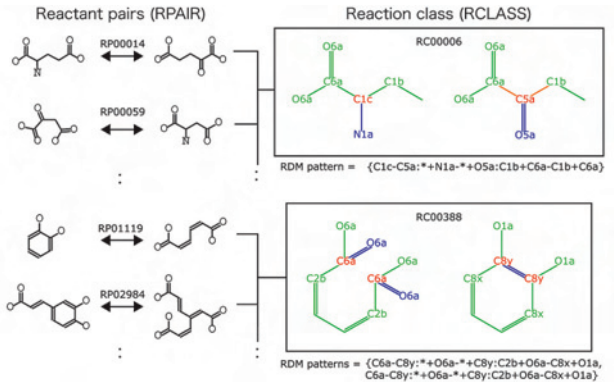

Figure 1. Example RCLASS entries and the RPAIR members.

PathPred: Enzyme-Catalyzed Reaction Pathway Prediction

PathPred is a newly developed web tool to predict plausible multi-step enzyme-catalyzed reaction pathways from a query compound using the information of the biochemical transformation patterns (RDM patterns) and chemical structure alignments of substrate-product pairs. PathPred provides transformed compounds and reference transformation patterns in each predicted reaction, and displays all predicted multi-step reaction pathways in a tree-shaped graph. This prediction server focuses on microbial biodegradation of environmental compounds and biosynthesis of plant secondary metabolites.

PathPred is a fully automatic server repeating prediction cycles until they reach the pre-specified compound, which is given by the user or is a compound present in the KEGG metabolic pathway maps. Another unique feature of PathPred is its potential to link the prediction result to genomic information. The PathPred server reports new and alternative reaction steps irrespective of whether enzymes for these steps are known or not. If the enzyme is not known, the E-zyme tool may be used to assign a possible EC number, which may then be used to search possible genes by sequence similarity of known genes.

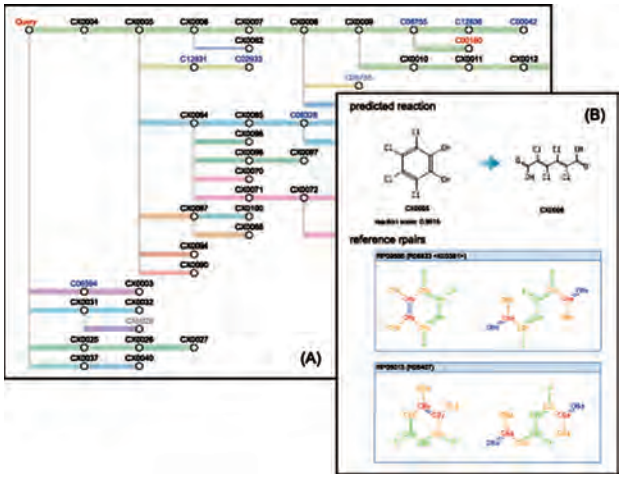

Figure 2. The example of the predicted pathway tree (A) and predicted reaction with referenced reactions.